AMENDMENTS TO THE CLAIMS

1. -11. (Cancelled)

12.   (New) A method for generating a shape signature representative of a molecular shape, the method comprising:

providing a visualization of a molecule formed of a plurality of atoms with a determined solvent-accessible molecular surface;

dividing said molecular surface into a plurality of small area elements;

performing a ray-trace on said visualization, said ray-trace comprising:

starting an initial ray segment at a start point in a first of said small area elements;

propagating said ray in a first direction until said ray impacts a second of said small area elements at an impact point;

recording characteristics of said ray segment;

repeating said starting, propagating, and recording for a new ray segment using said impact point of the prior iteration as said start point of the next iteration wherein said first direction associated with said new ray segment comprises the direction of reflection of said initial ray segment from said impact point;

stopping said repeating prior to recording if said first of said small area elements and said second of said small area elements are both on the same atom in said plurality of atoms;

if stopped, continuing said repeating by restarting the ray segment at said impact point of said prior iteration, but with a second direction different from said first direction; and

finishing said ray trace once a preselected number of ray segments have been recorded;

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computing a probability distribution based on characteristics of said ray, said probability

distribution providing an indication of said molecule's shape; and

storing said probability distribution indicative of said molecule's shape for later comparison

to other probability distributions indicative of other molecules' shape.